A MODEL FOR THERMO-HYDRO-MECHANICAL ANALYSIS OF MULTIPHASE POROUS MEDIA IN DYNAMICS

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Key words: Dynamics analysis, Variably saturated porous media, Non-isothermal problems, Thermo-hydro-mechanical coupling.

Abstract. This work presents the development of a mathematical and numerical model for the analysis of the thermo-hydro-mechanical behaviour of multiphase porous materials in dynamics. The fully coupled multiphase model for non-isothermal deformable porous media is developed within the Hybrid Mixture Theory. In order to analyse the thermo-hydro-mechanical behaviour of soil structures in the low frequency domain, e.g. under earthquake excitation, the u-p-T formulation is advocated neglecting the relative fluids acceleration and their convective terms. Moreover, the dynamic seepage forcing terms and the compressibility of the solid grain at the microscopic level are neglected. The standard Bubnov-Galerkin method is applied to the governing equations for the spatial discretization, whereas the generalized Newmark scheme is used for the time discretization. The final algebraic, non-linear and coupled system of equations is solved by the Newton method within the monolithic approach. The formulation and the implemented solution procedure are validated through the comparison with other finite element solutions or analytical solutions when available.

1 INTRODUCTION

The analysis of the dynamic response of multiphase porous media has many applications in civil engineering. Onset of landslide due to earthquake or rainfall and the seismic behaviour of earth dams are just few examples where inertial forces cannot be neglected because of the mass involved. Moreover, there are situations where it is important to consider the effect of temperature variation that causes a decrease of the solid skeleton strength and an increase of the pore water pressure. We could observe these phenomena for example during the onset of catastrophic landslide, as described in Vardoulakis [1], where the mechanical energy, dissipated in heat inside the slip zone, may also lead to the vaporization of pore water, creating a cushion of zero friction. Another example is the seismic behaviour of deep nuclear waste disposal, because an increment of temperature due to the failure of the canisters could create localized failure zones, which could act as preferential escape zones for the fluids containing radionuclides.

Many authors have developed models for the analysis of the dynamic behaviour of multiphase porous media in isothermal conditions. A state of art can be found in Zienkiewicz et al. [2] and Schanz [3]. Recently, Nenning and Schanz [4] presented an infinite element for wave propagation problems; Heider et al. [5] analyzed a numerical solution of dynamic wave propagation problems in infinite half spaces with incompressible constituents and Albers [6] analysed wave propagation problems in saturated and partially saturated porous media.

This work presents, as a novel contribution, a formulation of a fully coupled model for deformable multiphase geomaterials in dynamics including thermal effects.

The multiphase model is developed following Lewis and Schrefler [7]. The u-p-T formulation is obtained by neglecting the relative fluids acceleration and their convective terms, which is valid for low frequency problems as in earthquake engineering [2]. In the model devolvement, the dynamic seepage forcing terms in the mass balance equations and in the enthalpy balance equation and the compressibility of the grain at the microscopic level are neglected. The implemented model is validated through the comparison with analytical or finite element quasi-static and dynamic solutions.

2 MACROSCOPI BALANCE EQUATIONS

The full mathematical model necessary to simulate the thermo-hydro-mechanical behaviour of partially saturated porous media was developed within the Hybrid Mixture Theory by Lewis and Schrefler [7], Gawin and Schrefler [8] using averaging theories according to Hassanizadeh and Gray [9],[10]. The partially saturated porous medium is treated as multiphase system composed of the solid skeleton (s) and voids filled with liquid water (w) and gas (g); that the latter is assumed to behave as an ideal mixture of dry air (ga) and water vapour (gw). At the macroscopic level the porous material is modelled by a substitute continuum of volume B with boundary ∂B that simultaneously fills the entire domain, instead of the real fluids and the solid which fill only a part of it. In this substitute continuum each constituent π has a reduced density which is obtained through the volume fraction $\eta^{\pi}(\boldsymbol{x},t) = dv^{\pi}(\boldsymbol{x},t)/dv(\boldsymbol{x},t)$, where dv is the volume of the average volume element (representative elementary volume, REV) of the porous medium and dv_{π} is the volume occupied by the constituent π in dv. $\boldsymbol{x}$ is the vector of the spatial coordinates and t the current time.

The solid is deformable and non-polar, and the fluids, solid and thermal fields are coupled. The constituents are assumed to be isotropic, homogeneous, immiscible except for dry air and vapour, and chemically non-reacting. At micro level, solid is incompressible, while liquid water and gas are considered compressible. Local thermal equilibrium between solid matrix, gas and liquid phases is assumed. Heat conduction and convection, vapour diffusion, water flow due to pressure gradients or capillary effects and water phase change (evaporation and condensation) inside the pores are taken into account. In the partially saturated zones the liquid water is separated from its vapour by a meniscus concave toward gas. Due to the curvature of this meniscus the sorption equilibrium equation is assumed valid (for simplicity) and gives the relationship $p^c=p^g-p^w$ between the capillary pressure, gas pressure and liquid water pressure. The general field equations of the model are now written at macroscopic level in the geometrical linear setting.

The primary variables are chosen to be the displacements of the solid matrix, $\mathbf{u}(\boldsymbol{x},t)$, the capillary and gas pressure, $p^c(\boldsymbol{x},t)$ and $p^g(\boldsymbol{x},t)$, and the absolute temperature, $T(\boldsymbol{x},t)$.

The small terms related to relative accelerations of the fluids and their convective terms are neglected following [2]. This approximation is valid for dynamics at lower frequencies, as in earthquake engineering [2], [7], [11]. Dynamic seepage forcing terms connected with the solid acceleration are also neglected because their contribution is very small compared with other terms [2] (the effect of dynamic seepage can be of importance in the high frequency range where the **u**-p formulation is no longer valid [2]).

With the assumptions described above we obtain the **u**-p^c-p^g-T formulation of the balance equations to be implemented [12]:

Linear momentum balance equation of the mixture

$$div\boldsymbol{\sigma} + \rho\mathbf{g} = \rho\mathbf{a}^s \tag{1}$$

Water species (liquid and vapour) mass balance equation

$$\begin{aligned}
&\rho^w \frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} + \left[\rho^w S_w + \rho^{gw} S_g\right]\alpha div\mathbf{v}^s - \beta_{swg}\frac{\partial T}{\partial t} + n\left[\rho^w - \rho^{gw}\right]\frac{\partial S_w}{\partial t} + nS_g\frac{\partial \rho^{gw}}{\partial t} \\
&+ div\mathbf{J}_g^{gw} + div\left(\rho^w \frac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w + \rho^w\mathbf{g}\right]\right) + div\left(\rho^{gw}\frac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^{gw} + \rho^{gw}\mathbf{g}\right]\right) = 0
\end{aligned} \tag{2}$$

Dry air mass balance equation

$$\begin{aligned}
&S_g div\mathbf{v}^s + \frac{nS_g}{\rho^{ga}}\frac{\partial \rho^{ga}}{\partial t} + \frac{1}{\rho^{ga}}div\mathbf{J}_g^{ga} - n\frac{\partial S_w}{\partial t} \\
&+ \frac{1}{\rho^{ga}}div\left(\rho^{ga}\frac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^g + \rho^g\mathbf{g}\right]\right) + n\beta_s S_g\frac{\partial T}{\partial t} = 0
\end{aligned} \tag{3}$$

Enthalpy balance equation for the multiphase medium

$$\begin{aligned}
&\left(\rho C_p\right)_{eff}\frac{\partial T}{\partial t} - div\left(\chi_{eff}\, grad\, T\right) - \Delta H_{vap}\rho^w S_w \alpha div\mathbf{v}^s - \Delta H_{vap}\rho^w\frac{nS_w}{K_w}\frac{\partial p^w}{\partial t} \\
&+ \begin{bmatrix} \rho_w C_p^w nS_w \dfrac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w + \rho^w\mathbf{g}\right] \\ + \rho_g C_p^g nS_g\dfrac{k^{rg}\mathbf{k}}{\mu^g}\left[-gradp^g + \rho^g\mathbf{g}\right]\end{bmatrix} \cdot grad\, T + \Delta H_{vap}\beta_{sw}\frac{\partial T}{\partial t} \\
&- \Delta H_{vap} n\left[\rho^w - \rho^{gw}\right]\frac{\partial S_w}{\partial t} - div\left(\rho^w\frac{k^{rw}\mathbf{k}}{\mu^w}\left[-gradp^w + \rho^w\mathbf{g}\right]\right)\Delta H_{vap} = 0
\end{aligned} \tag{4}$$

The meaning of each variable of equations 1-4 are described in [7], [12] or [13].

3 CONSTITUTIVE RELATIONSHIP

For the gaseous mixture of dry air and water vapour, the ideal gas law is introduced. The equation of state of perfect gas (Clapeyron’s equation) and Dalton's law are applied to dry air (*ga*), water vapor (*gw*) and moist air (*g*).

In the partially saturated zones, the equilibrium water vapor pressure $p^{gw}(\boldsymbol{x},t)$ can be obtained from the Kelvin-Laplace equation, where the water vapor saturation pressure, p^{gws}, depending only upon the temperature, can be calculated from the Clausius-Clapeyron equation or from an empirical correlation. The saturation degree $S_\pi(\boldsymbol{x},t)$ and the relative permeability $k^{r\pi}(\boldsymbol{x},t)$ are experimentally determined functions.

The solid skeleton is assumed elastic, homogeneous and isotropic in the numerical simulations described in Section 5.

4 SPATIAL AND TIMES DISCRETIZATION

The finite element model is derived by applying the Galerkin procedure for the spatial integration and the Generalized Newmark Method for the time integration of the weak form of the balance equations of the previous section [2], [7], [14]. In particular, after spatial discretization within the isoparametric formulation, the following non-symmetric, non-linear and coupled system of equations is obtained [12]:

$$\begin{aligned}
&\int_\Omega \mathbf{B}^{\mathrm{T}}\boldsymbol{\sigma}'\,d\Omega - \mathbf{Q}\overline{\mathbf{p}}^g + \mathbf{R}\overline{\mathbf{p}}^c + \mathbf{M}\ddot{\overline{\mathbf{u}}} = \mathbf{f}_u \\
&\mathbf{U}\dot{\overline{\mathbf{p}}}^g + \mathbf{S}\dot{\overline{\mathbf{p}}}^c + \mathbf{T}\dot{\overline{\mathbf{T}}} + \mathbf{Q}'\dot{\overline{\mathbf{u}}} - \mathbf{I}\overline{\mathbf{p}}^g + \mathbf{H}\overline{\mathbf{p}}^c + \mathbf{E}\overline{\mathbf{T}} = \mathbf{f}_w \\
&\mathbf{S}'\dot{\overline{\mathbf{p}}}^c - \mathbf{T}'\dot{\overline{\mathbf{T}}} + \mathbf{R}'\dot{\overline{\mathbf{u}}} + \mathbf{I}'\overline{\mathbf{p}}^g - \mathbf{H}'\overline{\mathbf{p}}^c - \mathbf{E}'\overline{\mathbf{T}} = \mathbf{f}_g \\
&\mathbf{T}''\dot{\overline{\mathbf{T}}} - \mathbf{U}'\dot{\overline{\mathbf{p}}}^g + \mathbf{S}''\dot{\overline{\mathbf{p}}}^c - \mathbf{Q}''\dot{\overline{\mathbf{u}}} + \mathbf{E}''\overline{\mathbf{T}} - \mathbf{I}''\overline{\mathbf{p}}^g + \mathbf{H}''\overline{\mathbf{p}}^c = \mathbf{f}
\end{aligned} \tag{5}$$

where the displacements of the solid skeleton $\mathbf{u}(\boldsymbol{x},t)$, the capillary pressure $p^c(\boldsymbol{x},t)$, the gas pressure $p^g(\boldsymbol{x},t)$ and the temperature $\mathbf{T}(\boldsymbol{x},t)$ are expressed in the whole domain by global shape function matrices $\mathbf{N}_u(\mathbf{x}), \mathbf{N}_c(\mathbf{x}), \mathbf{N}_g(\mathbf{x}), \mathbf{N}_T(\mathbf{x})$ and the nodal value vectors $\overline{\mathbf{u}}(t), \overline{\mathbf{p}}^c(t), \overline{\mathbf{p}}^g(t), \overline{\mathbf{T}}(t)$. Following the Generalized Newmark Method, equations (5) are rewritten at time t_{n+1}.

After time integration, the non-linear system of equation is linearized, thus obtaining the equation system that can be solved numerically:

$$\mathbf{G}(\mathbf{x}_{i+1}) \cong \mathbf{G}(\mathbf{x}_i) + \left.\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right|_{x=x_i} d\mathbf{x}_i \cong 0 \tag{6}$$

where $\mathbf{x} = \left[\Delta\ddot{\overline{\mathbf{u}}} \quad \Delta\dot{\overline{\mathbf{p}}}_c \quad \Delta\dot{\overline{\mathbf{p}}}_g \quad \Delta\dot{\overline{\mathbf{T}}}\right]_{n+1}$ is the vector of the unknown, $\mathbf{G} = \left[\mathbf{G}^u \quad \mathbf{G}^w \quad \mathbf{G}^g \quad \mathbf{G}^T\right]_{n+1}$ and $\partial\mathbf{G}/\partial\mathbf{X}$ is the Jacobian matrix. Finally, the solution vector is updated by the incremental relationship $\mathbf{X}_{n+1}^{i+1} = \mathbf{X}_{n+1}^{i} + \Delta\mathbf{X}_{n+1}^{i+1}$.

5 VALIDATION AND APPLICATION EXAMPLES

In the following the numerical validation of the finite element model is presented by solving two numerical tests [12].

5.1 Numerical validation of the non-isothermal water saturated model

This problem deals with a fully saturated thermo-elastic consolidation problem [15], simulating a column, 7 m high and 2 m wide, of a linear elastic material subjected to an external surface load of 1000 Pa and to a surface temperature jump of 50 K above the initial temperature of 293.15 K (Figure 1). The material parameters used in the computation are summarised in [16]. The liquid water and the solid grain are assumed incompressible for the static analysis, whereas the compressibility of the liquid water is taken into account in the dynamic analysis. For the numerical calculation, the problem is solved as a two-dimensional problem in plane stain condition. The column is discretized with eight-node isoparametric elements (4 elements/meter); nine Gauss points are used.

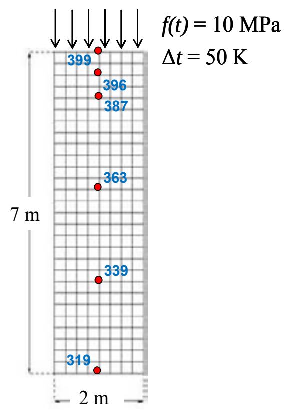

Figure 1: Geometry, loading conditions and finite element discretization of the saturated soil column

The initial and boundary conditions are described in Table 1.

Table 1: Initial and boundray conditions

Initial condition		Boundary condition	
P^g = Patm	fixed	P^g = Patm	fixed
P^c = idrostatic		P^c = 0.0	at the top
T = 293.15 K	fixed	T	not fixed
u_x = 0.0	on the lateral nodes	u_x = 0.0	on the lateral nodes
u_y = 0.0	on the bottom	u_y = 0.0	on the bottom

The solution of the finite element model presented in this work is compared with the quasi-static solution [16] and is plotted in Figures 2-4.

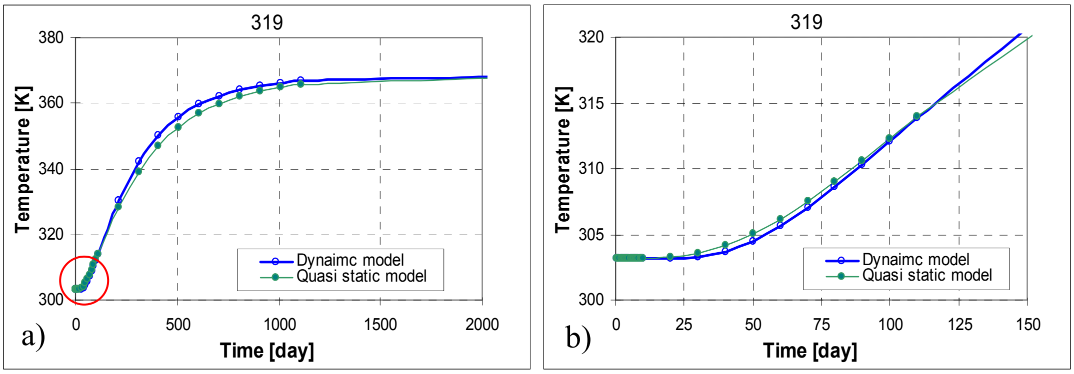

Figure 2: Temperature time history for node 319 up to the steady state solution (a) and in the first period (b) highlighted in a)

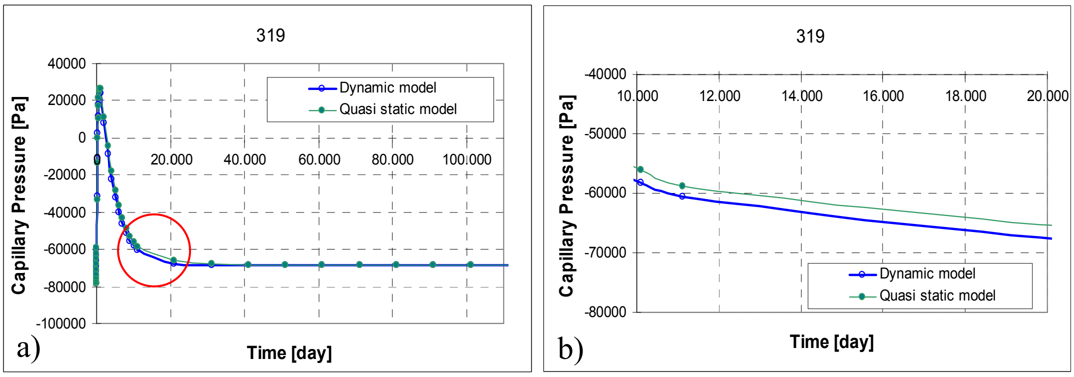

Figure 3: Capillary pressure time history for node 319 up to the steady state solution (a) and (b) during the time highlighted in a)

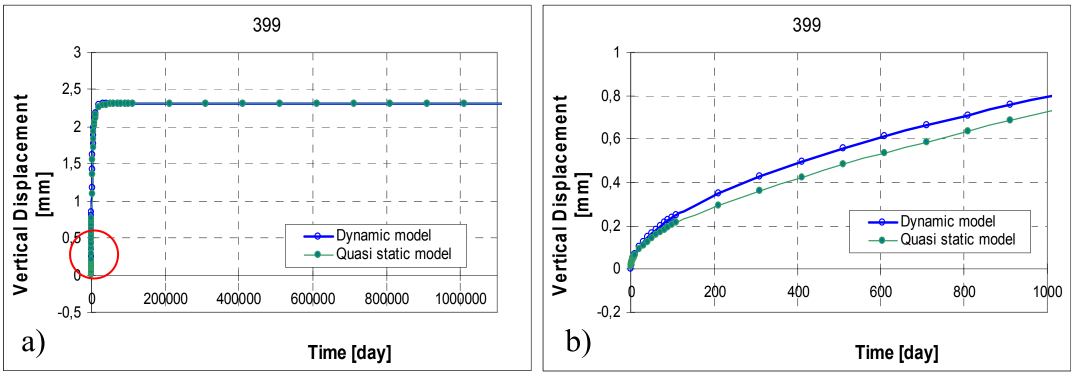

Figure 4: Vertical displacement time history for node 319 up to the steady state solution (a) and in the first period (b) highlighted in a)

It can be observed that the dynamic solution is faster than the quasi-static one at the beginning of the analysis, and that, at the end of the analysis, the dynamic solution reaches the quasi-static one.

5.2 Drainage of liquid water from initially water saturated soil column

The proposed benchmark is based on an experiment performed by Liakopoulos [17] on a column, 1 meter high, of Del Monte sand and instrumented to measure the moisture tension at several points along the column during its desaturation due to gravitational effects. Before the start of the experiment, water was continuously added from the top and was allowed to drain freely at the bottom through a filter, until uniform flow conditions were established. Then the water supply was ceased and the tensiometer readings were recorded. The finite element simulation is performed with the two-phase flow model in isothermal conditions, with switching between saturated and unsaturated solution performed at p^c= 2000 Pa (S_w= 0,998), which corresponds to bubbling pressure of the analysed sand, and an additional lower limit for the gas relative permeability of 0,0001 [8]. For the numerical calculation, a two-dimensional problem in plane strain conditions is solved; the spatial domain of the column is divided into 20 eight-node isoparametric finite elements of equal size. Furthermore, nine Gauss integration points were used. The material parameters are listed in [8] or [20].

This problem has been solved considering single or two-phase flow mainly in quasi-static condition; a finite element solution in dynamics was presented in [18]. The initial hydro-mechanical equilibrium state is obtained via a preliminary quasi-static solution. The initial and boundary conditions for the dynamic analysis are summarized in Table 2.

Table 2: Initial and boundary conditions

Initial condition		Boundary condition	
P^g = Patm	on the top	P^g = Patm	on the top, on the bottom
P^c = idrostatic		P^c = 0.0	on the bottom
T = 293.15 K	fixed	T = 293.15 K	fixed
u_x = 0.0	on the lateral nodes	u_x = 0.0	on the lateral nodes
u_y, V_y = 0.0	on the bottom	u_y = 0.0	on the bottom

The comparison between the dynamic and the quasi-static solution is plotted in Figures 5-7, where the profiles for water pressure, water saturation and vertical displacement along the column are plotted. Since the inertial loads are negligible in the experiment, the finite element solution in dynamics gives almost the same results of the quasi-static solution (Figures 5b-7b).

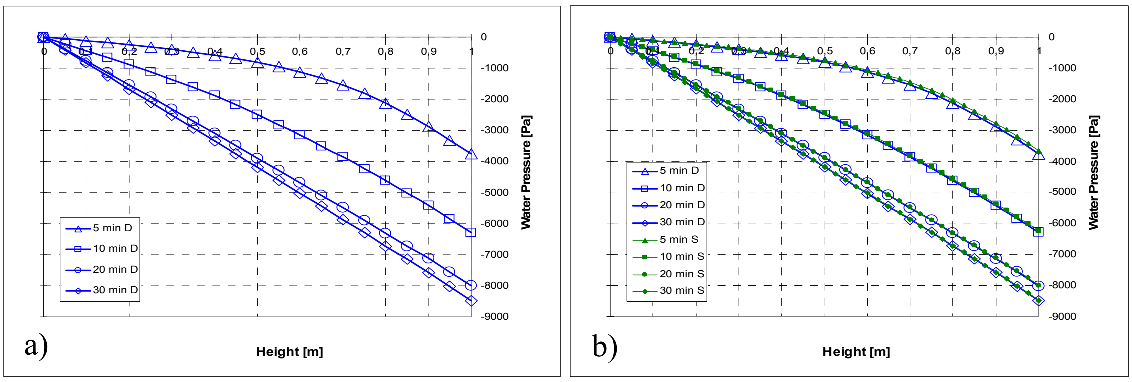

Figure 5: Profiles of water pressure versus height (a – dynamic solution) and comparison between the quasi-static (S) and the dynamic solution (D) at 5, 10, 20 and 30 minutes (b)

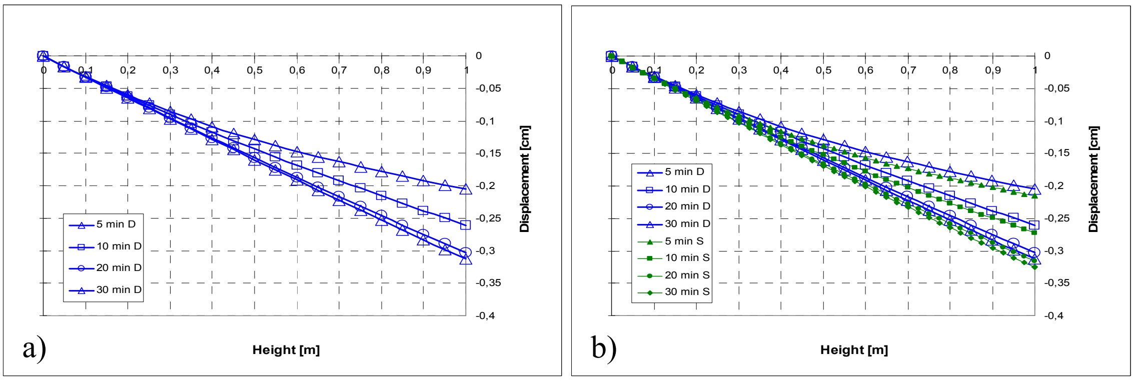

Figure 6: Profiles of vertical displacement versus height (a – dynamic solution) and comparison between the quasi-static (S) and the dynamic solution (D) at 5, 10, 20 and 30 minutes (b)

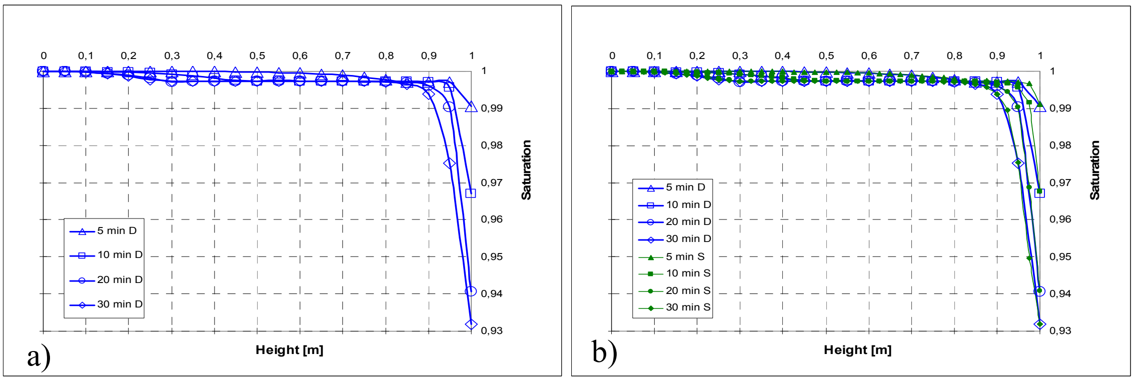

Figure 67 Profiles of saturation versus height (a – dynamic solution) and comparison between the quasi-static (S) and the dynamic solution (D) at 5, 10, 20 and 30 minutes (b)

7 CONCLUSIONS

A model for the analysis of the thermo-hydro-mechanical behaviour of porous media in dynamics was developed. Starting from the generalized mathematical model developed by Lewis and Schrefler [7] for deforming porous media in non-isothermal conditions, the u-p-T formulation was derived following [2]. The validity of such an approximation is limited to low frequencies problems [2], as in earthquake engineering. In this formulation the relative accelerations of the fluids and the convective terms related to these accelerations are neglected. Moreover, in the model development, the compressibility of the solid grain at microscopic level and the dynamic seepage forcing terms were neglected.

The numerical model was derived within the finite element method: the standard Bubnov-Galerkin procedure [14] was adopted for the discretization in space, while the implicit and unconditionally stable Newmark procedure was applied for the discretization in time [14]. The independent variables chosen are: the displacement of the solid skeleton **u**, the capillary pressure p^c, the gas pressure p^g and the temperature T.

The model was implemented in the finite element code Comes-Geo [7], [8], [13], [16], [19], [20], [21], [22]. The formulation and the implemented solution procedure were validated through the comparison with literature benchmarks, finite element solutions or analytical solutions [12]. In this paper, comparison between the finite element solution in dynamics and the corresponding quasi-static solution is presented by studying the non-isothermal consolidation in a water saturated column and the drainage of liquid water in an initially water saturated soil column.

This work extends the model developed in [18] to non-isothermal conditions and removes the passive air phase assumption of the multiphase porous media model in dynamics developed in [2], [23], [24], [25] and used in [26] to study the seismic behaviour of an earth dam.

ACKNOWLEDGEMENTS

The authors would like to thank the University of Padua for financial support (projects: CPDA097373 and STPD08JA32).

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